

Virtual ligand screening studies between mushroom compounds and proteins involved in breast cancer

H. J.C. Froufe, R. M. V. Abreu, I. C.F.R. Ferreira*

CIMO- ESA, Instituto Politécnico de Bragança, Campus de Santa Apolónia, apartado 1172, 5301-855 Bragança, Portugal

* e-mail: iferreira@ipb.pt; telefone +351-273-303219; fax +351-273-325405

Mushrooms are a vast and yet largely untapped source of powerful new pharmaceutical products. In particular, and most importantly for modern medicine, they represent an unlimited source of compounds with antitumor and immunostimulating properties [1]. Particularly, the intake of some wild mushrooms has shown to reduce the risk of breast cancer in Chinese women [2]. A large number of LMW (low molecular weight) compounds have been identified in wild mushrooms including phenolic acids, flavonoids, tocopherols, carotenoids, sugars and fatty acids [3]. In this study we used AutoDock 4 [4] to perform virtual ligand screening in order to evaluate which LMW compounds may be involved in the inhibition of the activity of proteins related to human breast cancer: aromatase (EC: 1.14.14.1), estrone sulfatase (EC: 3.1.6.2) and 17-hydroxysteroid dehydrogenase type 1 activity (17 β -HSD-1; EC: 1.1.1.62) [5]. A representative dataset of 43 LMW compounds was selected and molecular docking was performed against the three protein targets. 4-*O*-caffeoylquinic, naringin and lycopene stand out as the top ranked potential inhibitors for aromatase, estrone sulfatase and 17 β -HSD1, respectively. The information provided shows several interesting starting points for further development of inhibitors of the studied proteins, as also for the development of nutraceuticals or functional foods.

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References:

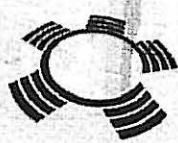
- [1] Zaidman B., Yassin M., Mahajana J., Wasser S.P. (2005). *Applied Microbiology and Biotechnology* 67, 453-468.
- [2] Zhang M., Huang J., Xie X., Holman C.D.J. (2009). *International Journal of Cancer* 124, 1404-1408.
- [3] Ferreira I.C.F.R., Barros L., Abreu R.M.V. (2009). *Current Medicinal Chemistry* 16, 1543-1560.
- [4] Morris G.M., Goodsell D.S., Halliday R.S., Huey R., Hart W.E., Belew R.K., Olson A.J. (1998). *Journal of Computational Chemistry*, 19, 1639-1662.
- [5] Pasqualini J.R., Chetrite G.S. (2005). *Journal of Steroid Biochemistry and Molecular Biology* 93, 221-236.



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CERTIFICADO

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